MULTISCALE SIMULATION OF DEFECTS USING MULTIGRID ATOMISTIC CONTINUUM METHOD

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A method to simulate the behavior of defects in 3D in crystalline materials using multiscale technique is presented here. The method finds applications in modeling of nanostructures such as electronic materials, thin film growth etc. In this method atomistic representation is used in regions of high field gradients or where the highly non-linear and an non-local behavior of the lattice is important, while continuum is used elswhere. This method has the benefit of utilizing all the developed tools and codes of the finite element method, such as higher order elements, error estimation, adaptivity etc, while combining them with the tools developed for atomistic analysis.

In this method, the continuum is discretized using finite elements on a coarse grid. Defects are represented atomistically only during nucleation or close range interaction. In these regions, a fine grid is used which carries the boundary conditions imposed by the continuum and returns to the continuum correcting eigenstrains. Appropriate interpolation operators are used for this linkage. Hence, the discrete grid is defined in restricted spatial regions and relocates with the defects. Defects which are not in close range interaction are represented by means of their continuum elastic field as in discrete dislocation dynamics simulations. This procedure minimizes the computational effort associated with atomistic simulations, while insuring the required accuracy at relevant spatial locations. This method doesn't have the restriction of matching atomistic and continuum grids as in the method described in [1]. Figure 1 gives a schematic description of the method.

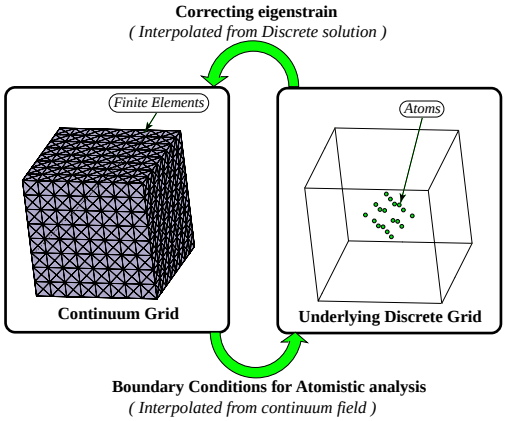

Figure 1: A schematic description of the method. The discrete grid is placed at the site of the defect.

Several test examples which demonstrates the coupling of the method will be given. The method will then be applied to simulate the crack propagation process of f.c.c. crystalline materials which tracks evolving and interacting dislocations.

References

[1] S. Kohlhoff, P. Gumbsch, and H.F. Fishchmeister, "Crack propagation in b.c.c. crystals studied with a combined finite-element and atomistic model", *Philosophical Magazine A*, v. 64, p. 851-878, 1991.